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Entropy of Mixing and Binary Nucleation Kinetics[1] Gerald Wilemski, Lawrence Livermore National Laboratory, Livermore CA 94551-9900.

Most research on binary nucleation has employed the capillarity approximation because of the lack of a satisfactory molecular theory. The capillarity approximation treats the free energy of the critical nucleus as a sum of volume and surface terms, with each term evaluated using bulk material properties. The fundamental inadequacy of this classical approach has long been appreciated. Generally, any deficiency of the classical theory of binary nucleation is attributed to the surface free energy term. However, there is also a defect in the theory stemming from inadequate consideration of the entropy of mixing contribution to the cluster free energy. This defect results in several kinds of unphysical behavior, but it can be remedied by taking into account the finite size of the cluster when computing its entropy of mixing. This will be illustrated using results for a simple, exactly solvable model of binary nucleation.

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